

Reinvent 4: Modern AI–driven generative molecule design

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Abstract

REINVENT 4 is a modern open-source generative AI framework for the design of small molecules. The software utilizes recurrent neural networks and transformer architectures to drive molecule generation. These generators are seamlessly embedded within the general machine learning optimization algorithms, transfer learning, reinforcement learning and curriculum learning. REINVENT 4 enables and facilitates de novo design, R-group replacement, library design, linker design, scaffold hopping and molecule optimization. This contribution gives an overview of the software and describes its design. Algorithms and their applications are discussed in detail. REINVENT 4 is a command line tool which reads a user configuration in either TOML or JSON format. The aim of this release is to provide reference implementations for some of the most common algorithms in AI based molecule generation. An additional goal with the release is to create a framework for education and future innovation in AI based molecular design. The software is available from <https://github.com/MolecularAI/REINVENT4> and released under the permissive Apache 2.0 license. Scientific contribution. The software provides an open–source reference implementation for generative molecular design where the software is also being used in production to support in–house drug discovery projects. The publication of the most common machine learning algorithms in one code and full documentation thereof will increase transparency of AI and foster innovation, collaboration and education.